Monte Carlo Simulation of Miscibility of Polymer Blends

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A newly proposed simulation method, Hyper-Parallel Tempering Monte Carlo, has been applied to investigate the phase behavior (miscibility) of highly asymmetric polymer blends on a lattice. The simulations have been performed in the grand-canonical ensemble; density fluctuations and compressibility are therefore consider explicitly in our calculations. The new method is powerful enough to permit study of blends of long polymers at elevated densities.

In this work we have examined the effect of energetic asymmetry, molecular-weight difference, flexibility difference, and branching on the miscibility of binary blends. The results of our simulations are compared to available theoretical formalisms for description of the thermodynamic properties of such systems. Our results are also compared to those of earlier simulations for smaller systems.